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1 Abstract

Flame structure and ignition and extinction processes associated with a strained fuel strip are explored numerically using detailed transport and complex kinetics for a propane-air reaction. Ignition modes are identified that are similar to those predicted by one-step activation energy asymptotics, i.e., modes in which diffusion flames can ignite as independent or dependent interfaces, and modes in which single premixed or partially premixed flames ignite. These ignition modes are found to be dependent on critical combinations of strain rate, fuel strip thickness, and initial reactant temperatures. Extinction in this configuration is seen to occur due to fuel consumption by adjacent flames, although viscosity is seen to have the effect of delaying extinction by reducing the effective strain rate and velocity field experienced by the flames.

2 Introduction

Ignition and extinction processes associated with a single strained fuel-air interface have been examined extensively over the years using single step activation energy asymptotics[1–4] as well as reduced kinetics simulation[5–7] and full combustion chemistry simulation[8, 9]. These processes may be understood in terms of the classical “S-shaped curve”[2, 3, 10], representing the thermal runaway leading to ignition as strain rate is relaxed and flame extinction as strain rate is increased. The concept of ignition delay due to straining has been applied to a variety of situations, including an understanding of flame liftoff[4, 11] as well as ignition delay processes in jets, shear layers, and vortical structures[6, 12–14].

In many complex flow situations, strained fuel-air interfaces form[15] and are brought closely together into layer-like turbulent flow structures which may be viewed as alternating fuel-oxidizer strips undergoing local strain. These dissipation and reaction layers are comprised of laminar “flamelets” which are used to model turbulent non-premixed combustion[16]; it has been suggested that the existence of these layers is independent of the extent of chemical non-equilibrium in the flow[17].

While extinction of the interfaces bounding finite regions of fuel has been considered in the fast chemistry limit[18, 19] as well as using finite rate single step kinetics[20] due to fuel burnout, the interesting problem of ignition delay associated with a strained fuel layer, bounded by oxidizing species, has only recently been studied via single step activation

energy asymptotics[21]. This study examined how the ignition process is affected as strained interfaces are brought closely together due to straining. Three possible modes of ignition are determined: one in which the two interfaces ignite independently to form diffusion flames, one in which the two interfaces ignite in a dependent fashion and in which ignition may be actually augmented by strain due to enhanced thermal feedback, and one in which ignition occurs to form a single, premixed flame at very high strain rates before ignition is completely prevented. In contrast to a single, isolated interface in which ignition can be prevented by over-matching heat production with heat convection due to strain, ignition of a strained fuel strip can also be prevented if the finite extent of fuel is diluted by oxidizer more quickly than heat production can cause a positive feedback thermal runaway. These behaviors are dependent on the relative sizes of time scales associated with species and heat diffusion, with convection due to strain, and with the chemical reaction. Critical strain rates leading to complete ignition delay can be considerably smaller for the fuel strip than those for single interfaces as the fuel strip is made thin in comparison to diffusion and chemical length scales.

When critical strain rates leading to ignition prevention for two adjacent species interfaces are smaller than those required to delay ignition of a single isolated interface, certain benefits may be derived. If ignition is delayed due to strain in a turbulent reactive flow, fuel and air can experience substantial mixing, so that when the strain field relaxes, ignition may occur in a premixed mode, potentially reducing NO_x production that would occur in stoichiometric diffusion flames[22]). The strained fuel strip is in fact a component of a low NO_x, lobed fuel injector currently under examination[23, 24]. Streamwise vorticity generated by the injector creates a flowfield of high strain, acting to delay the ignition of injected strips of fuel into a coflowing airstream. These issues are what motivated the earlier study of ignition delay in strained fuel layers via activation energy asymptotics[21]; they continue to motivate the present, more quantitative study which examines ignition, burning, and extinction in a propane fuel strip surrounded by air using a full kinetic mechanism.

3 Problem Formulation and Solution Procedure

The geometry of the strained fuel strip problem is shown in Figure 1. The strain rate imposed in the problem is formulated through boundary conditions as $y \rightarrow +\infty$, that is, $u(x, y \rightarrow +\infty, t) = \epsilon x$ and $v(x, y \rightarrow +\infty, t) = -\epsilon y$. It should be noted that the boundary conditions as $y \rightarrow -\infty$ are the same as those as $y \rightarrow +\infty$ due to the presence of air in both limits, in contrast to the classical counterflow diffusion flame problem with differing initial densities of fuel and air. The strained fuel strip problem is actually richer from a phenomenological point of view than is ignition of the single diffusion flame in that additional modes of ignition are possible, as noted in [21].

The governing equations for the strained fuel strip problem (mass, momentum, energy, and species conservation) may be solved in general in the present scheme in conservative form:

$$\vec{U}_t + [\vec{F}(\vec{U})]_x + [\vec{G}(\vec{U})]_y = [\vec{F}_v(\vec{U})]_x + [\vec{G}_v(\vec{U})]_y + \vec{S} \quad (1)$$

where the vector \vec{U} (containing the density ρ , velocity components u and v , energy per unit volume e , pressure p , and mass fractions Y_i), the convective flux vectors \vec{F} and \vec{G} , the diffusive flux vectors \vec{F}_v and \vec{G}_v , and the source vector \vec{S} are defined as follows:

$$\vec{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho Y_1 \\ \rho Y_2 \\ \vdots \\ \rho Y_{NS-1} \end{pmatrix} \quad \vec{F}(\vec{U}) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (e+p)u \\ \rho u Y_1 \\ \rho u Y_2 \\ \vdots \\ \rho u Y_{NS-1} \end{pmatrix} \quad \vec{G}(\vec{U}) = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (e+p)v \\ \rho v Y_1 \\ \rho v Y_2 \\ \vdots \\ \rho v Y_{NS-1} \end{pmatrix} \quad (2)$$

$$\vec{F}_v(\vec{U}) = \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ u\tau_{xx} + v\tau_{xy} + Q_x \\ \rho D_{1m}(Y_1)_x \\ \rho D_{2m}(Y_2)_x \\ \vdots \\ \rho D_{NS-1m}(Y_{NS-1})_x \end{pmatrix} \quad \vec{G}_v(\vec{U}) = \begin{pmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ u\tau_{xy} + v\tau_{yy} + Q_y \\ \rho D_{1m}(Y_1)_y \\ \rho D_{2m}(Y_2)_y \\ \vdots \\ \rho D_{NS-1m}(Y_{NS-1})_y \end{pmatrix} \quad (3)$$

$$\vec{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \dot{\omega}_1 \\ \dot{\omega}_2 \\ \vdots \\ \dot{\omega}_{NS-1} \end{pmatrix} \quad (4)$$

Mass production rate terms $\dot{\omega}_i$ are evaluated in (4) in standard fashion, assuming an Arrhenius-type reaction rate coefficient dependence on temperature. Inviscid as well as viscous forms of the equations have been solved in one and two dimensions, respectively[25].

If a one-dimensional formulation is made and if pressure is assumed spatially invariant, as done by Darabiha[26] and by Petrov and Ghoniem[27], for example, with the simplified boundary conditions, the problem essentially reduces to a set of energy and species conservation equations:

$$\vec{U}_t + [\vec{G}(\vec{U})]_y = + [\vec{G}_v(\vec{U})]_y + \vec{S} + \vec{C} \quad (5)$$

where

$$\vec{U} = \begin{pmatrix} e \\ \rho Y_1 \\ \rho Y_2 \\ \vdots \\ \rho Y_{NS} \end{pmatrix} \quad \vec{G}(\vec{U}) = \begin{pmatrix} (e+p)v \\ \rho v Y_1 \\ \rho v Y_2 \\ \vdots \\ \rho v Y_{NS} \end{pmatrix} \quad \vec{G}_v(\vec{U}) = \begin{pmatrix} Q_y \\ \rho D_{1m}(Y_1)_y \\ \rho D_{2m}(Y_2)_y \\ \vdots \\ \rho D_{NS,m}(Y_{NS})_y \end{pmatrix} \quad (6)$$

and

$$\vec{S} = \begin{pmatrix} 0 \\ \dot{\omega}_1 \\ \dot{\omega}_2 \\ \vdots \\ \dot{\omega}_{NS} \end{pmatrix} \quad \vec{C} = \begin{pmatrix} -\epsilon(e+p) \\ -\epsilon \rho Y_1 \\ -\epsilon \rho Y_2 \\ \vdots \\ -\epsilon \rho Y_{NS} \end{pmatrix} \quad (7)$$

where the heat flux component, neglecting radiative heat transfer, is given by:

$$Q_y = \lambda T_y + \rho \sum_{k=1}^{NS} h_k D_{km}(Y_k)_y \quad (8)$$

The above equations may be solved numerically. The energy conservation equation is solved in terms of the energy per unit volume e (or actually, the enthalpy per unit mass, h). This is in *contrast* to the common assumption of a “locally” calorically perfect gas where $h = \bar{c}_p T$ is assumed in the governing equations, employing table look-ups to obtain the dependence of $c_{p,i}$ for each species on temperature in the governing equation and averaging to obtain \bar{c}_p . While for many combustion problems the usual approach yields accurate results, it has been recently shown[29] that such assumptions in the vicinity of sharp gradients such as flames can yield errors in wave speeds and hence in the solution of the problem. The present approach avoids this difficulty.

Formulation of the ratio of specific heats for the mixture of gases present in a given computational cell is done so as to avoid thermodynamic inconsistencies at contact discontinuities. These inconsistencies are known to generate temperature spikes and numerical oscillations[30–32]. In the present procedure we use the relation

$$\gamma = 1 + \frac{\sum_{k=1}^{NS} \frac{Y_k}{W_k}}{\sum_{k=1}^{NS} \frac{Y_k}{W_k(\gamma_k - 1)}} \quad (9)$$

for the ratio of specific heats of the gas mixture in a given cell; this assumes that all species Y_k with molecular weights W_k are at the same temperature within the cell. Although this assumption is not as accurate as evolving γ from partial pressures of the species, as done by Ton[30], experience has shown that if a sharp contact surface rapidly fades away due to the presence of highly diffusive species, then using equation (9) will result in confined spikes in temperature for only very short periods of time.

The method of Strang splitting or operator splitting via fractional steps[33] is employed to solve the system of equations (1) or (5). This procedure enables the system to be split into two separate equations, one which only includes the advection-diffusion terms and one which only includes the reaction rate source terms, respectively:

$$\vec{U}_t + [\vec{F}(\vec{U})]_x + [\vec{G}(\vec{U})]_y = [\vec{F}_v(\vec{U})]_x + [\vec{G}_v(\vec{U})]_y \quad (10)$$

$$\vec{U}_t = \vec{S} \quad (11)$$

An equivalent form of equations (10) and (11) may be written for the inviscid formulation of the problem, equation (5). Each relation above represents a set of equations that has been studied extensively. The present method uses a first-order upwind scheme[34] to solve the inviscid form of the advection-diffusion equation (10) and the second-order McCormack predictor-corrector scheme[36] to solve (10) in the full viscous form. It employs a stiff ODE solver (VODE[35], an improved version of LSODE[37]) accompanied by the CHEMKIN-II package[38] to solve equation (11).

The above formulation has been demonstrated to be relatively efficient as well as accurate in its prediction of the structure of strained diffusion flames and fuel strips. The present calculation employs the propane-air chemical mechanism of [39] to study ignition, burning, and extinction of a strained propane fuel strip.

4 Results

Results for the ignition, burning, and extinction processes associated with the propane strip burning in air are shown in Figures 2-6 for the inviscid case. Figure 2 is a plot of temperature as a function of distance across the fuel strip and as a function of time, for a fuel strip ($T = 400^\circ \text{ K}$) of initial thickness 1 mm in heated air ($T = 1300^\circ \text{ K}$) in the absence of straining. For this relatively thick fuel strip, ignition occurs at two distinct locations in an independent manner. Burning proceeds by each flame in an independent manner as well, evidenced by movement of each flame toward the adjacent oxidizer, in accordance with the stoichiometric requirements of the reaction. This ignition mode is consistent with the asymptotic analysis of ignition in [21] whereby relatively thick fuel strips at zero or low rates of strain ignite independently. Figure 2 demonstrates that the interfaces burn in an independent fashion as well prior to the beginning of fuel burnout.

Figure 3, in contrast, shows the evolution of temperature field associated with a fuel strip of the same initial thickness as in Figure 2 but exposed to a constant strain rate of 500 sec^{-1} . While only a slight delay in ignition is observed in comparison to that in Figure 2, there is a very clear interdependence of the flames that do ignite; the flames then proceed to move toward each other, rapidly depleting the intervening fuel and extinguishing at a short time later. This behavior is a quantitative confirmation of the enhancement of thermal feedback suggested by the single step asymptotic solution of this ignition problem[21] and the corresponding dependent ignition mode for the fuel-air interfaces. The rapid burnout

process is further demonstrated by plots of propane, OH, and H radical mass fractions as a function of space and time shown in Figure 4. The figure also demonstrates that the runaway in the H radical can precede the runaway in temperature during ignition of the interfaces, similar to the observations of Kreutz, *et al.*[9] for single strained fuel-air interfaces.

Figures 5 and 6 show plots of temperature, propane, OH, and H radical mass fractions as a function of space and time for the propane fuel strip of the same initial thickness as above but with successively higher constant rates of strain. In Figure 5 there is a greater ignition delay than in Figure 4, but with ignition at a single location, indicating that ignition and sustained burning occur in the premixed or partially premixed mode. Here the rate of strain is so high that the fuel-air interfaces are brought together very rapidly, and substantial interchange of mass occurs before the ignition process. This mode of ignition again is a quantitative confirmation of the single ignition mode observed in the single-step asymptotic solution of this problem[21]. As is expected, this flame consumes the existing fuel-air mixture and burns out very rapidly. Figure 6, at a constant strain rate of 1500 sec^{-1} , demonstrates that at extremely high rates of strain, ignition can be prevented in the strained fuel strip; no significant formation of radicals, rise in temperature, or fuel consumption occurs. This “non-ignition” mode occurs due to the very rapid mixing of fuel and air, so high that fuel is diluted beyond the level required for ignition of the mixture. This observation is also seen in the asymptotic solution of the problem[21], and differs from modes of ignition prevention seen for single fuel-air interfaces in which heat loss due to high strain prevents thermal runaway.

Finally, a sample result for solution of the viscous flow problem, equation (1), is shown in Figure 7a, with comparison made to the equivalent inviscid problem, equation (5), in Figure 7b. While the actual process of ignition and ignition times are the same for the two computations, the process of sustained burning of the fuel strip and eventual burnout is substantially longer for the viscous simulation than for the inviscid simulation. Clearly, the effect of viscosity is to reduce the effective velocity and strain field experienced by the species interfaces, transporting them more slowly toward each other and allowing for a reduced rate of consumption of intervening fuel.

5 Summary and Conclusions

The present study demonstrates that a full numerical simulation of ignition of a strained fuel strip with complete combustion chemistry exhibits the same phenomenological modes of thermal/radical runaway that are seen in a single-step asymptotic simulation of the problem. Further, burning and extinction processes may be explored via numerical simulation; these calculations suggest the sensitivity of the combustion characteristics to the degree of straining and the presence of viscosity in the flowfield.

6 Acknowledgements

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7 References

References

- [1] Fendell, F. E., *J. Fluid Mech.* 21 (Pt. 2): 281-303 (1965).
- [2] Liñan, A., *Acta Astronautica* 1: 1007-1039 (1974).
- [3] Liñan, A. and Crespo, A., *Combust. Sci. Tech.* 14: 95-117 (1976).
- [4] Peters, N., *Combust. Sci. Tech.* 30: 1-17 (1983).
- [5] Dold, J. W., *Combust. Flame* 76: 71-88 (1989).
- [6] Thévenin, D. and Candel, S., *Combust. Sci. Tech.* 91: 73-94 (1993).
- [7] Seshadri, K. and Peters, N., *Combust. Flame* 73: 23 (1988).
- [8] Darabiha, N. and Candel, S., *Combust. Sci. Tech.* 86: 67-85 (1992).
- [9] Kreutz, T. G., Nishioka, M., and Law, C. K., *Combust. Flame* 99: 758-766 (1994).
- [10] Law, C. K., *Twenty-second Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1988, pp. 1381-1402.
- [11] Peters, N., *Twenty-first Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1986, pp. 1231-1250.
- [12] Grosch, C. E. and Jackson, T. L., *Phys. Fluids A* 3: 3087-3097 (1991).
- [13] Macaraeg, M. G., Jackson, T. L., and Hussaini, M. Y., *Combust. Sci. Tech.* 87: 363-387 (1992).
- [14] Thévenin, D. and Candel, S., *Phys. Fluids* 7: 434-445 (1995).
- [15] Carrier, G. F., Fendell, F. E., and Marble, F. E., *SIAM J. Appl. Math.* 28: 463-500 (1975).
- [16] Peters, N., *Prog. Energy Combust. Sci.* 10: 319-339 (1984).
- [17] Bish, E. S. and Dahm, W. J. A., *Combust. Flame* 100: 457-466 (1994).

- [18] Marble, F. E., *Recent Adv. in Aero. Sci.*, C. Casci, Ed., pp. 395-413 (1985).
- [19] Buckmaster, J. D. and Ludford, G. S. S., *Theory of Laminar Flames*, Cambridge University Press, 1982, pp. 179-181.
- [20] Cetegen, B. M. and Bogue, D. R., *Combust. Flame* 86: 359-370 (1991).
- [21] Gerk, T. J. and Karagozian, A. R., "Ignition Delay Associated with a Strained Fuel Strip", to appear in the *Twenty-Sixth Symposium (International) on Combustion*, 1996.
- [22] Bowman, C. T., *Twenty-fourth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, 1992, pp. 859-878.
- [23] Smith, L. L., Majamaki, A. J., Lam, I. T., Delabroy, O., Karagozian, A. R., Marble, F. E., and Smith, O. I., "Mixing Enhancement in a Lobed Injector", submitted to *The Physics of Fluids*.
- [24] Mitchell, M. G., Smith, L. L., Karagozian, A. R., and Smith, O. I., "NO_x Emissions from a Lobed Fuel Injector/Burner", Paper 96F-075. Western States Section/The Combustion Institute Fall Meeting, October, 1996.
- [25] Selerland, T., "Numerical Simulation of Ignition, Burning, and Extinction Processes for Strained Flames", Ph.D. prospectus, UCLA, September, 1996.
- [26] Darabiha, N., "Transient Behaviour of Laminar Counterflow Hydrogen-Air Diffusion Flames with Complex Chemistry", *Combust. Sci. Tech.* 86: 163-181 (1992).
- [27] Petrov, C. A. and Ghoniem, A. F., "The Transient Response of Strained Laminar Premixed Flames", *Combustion and Flame*, Vol. 102, pp. 401-417 (1995).
- [28] Egolfopoulos, F. N., "Dynamics and Structure of Unsteady, Strained, Lamine Premixed Flames", *Twenty-fifth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, PA, pp. 1365-1373 (1994).
- [29] Fedkiw, R., "A Survey of Chemically Reacting, Compressible Flows", Ph.D. thesis, Department of Mathematics, UCLA, 1996.
- [30] Ton, V. T., "Improved Shock-Capturing Methods for Multicomponent and Reacting Flows" to appear in the *Journal of Computational Physics*, 1996.
- [31] Abgrall, R., "Generalization of the Roe Scheme for Computing Flows of Mixed Gases with Variable Concentrations", *La Recherche Aerospatiale*, Vol. 6, pp. 31-43 (1988).
- [32] Larrouturou, B., "How to Preserve the Mass Fractions Positivity when Computing Compressible Multi-component Flows", *Journal of Computational Physics*, Vol. 95, pp. 59-84 (1991).

- [33] Strikwerda, J. C., *Finite Difference Schemes and Partial Differential Equations*. Wadsworth and Brooks (1989).
- [34] LeVeque, R. J., *Numerical Methods for Conservation Laws*, Birkhauser, Basel (1992).
- [35] Brown, P. N., Byrne, G. D., and Hindmarsh, A. C., "VODE: A Variable Coefficient ODE Solver", *SIAM Journal of Scientific Statistical Computing*, Vol. 10, pp. 1038-1051 (1989).
- [36] MacCormack, R. W. (1969). "The effect of viscosity in hypervelocity impact cratering" AIAA Paper 69-354, AIAA, 1969.
- [37] Hindmarsh, A. C., "ODEPACK, a Systematized Collection of ODE Solvers", in *Scientific Computing*, R. S. Stepleman, *et al.*, eds., North-Holland, Amsterdam, pp. 55-64 (1983).
- [38] Kee, R. J., Miller, J. A., and Jefferson, T. H., "CHEMKIN: A General Purpose, Problem Independent, Transportable, Fortran Chemical Kinetics Code Package", Sandia National Laboratories Report SAND80-8003 (1980).
- [39] Warnatz, J., *Comb. Sci. and Tech.* 34: 177 (1983).

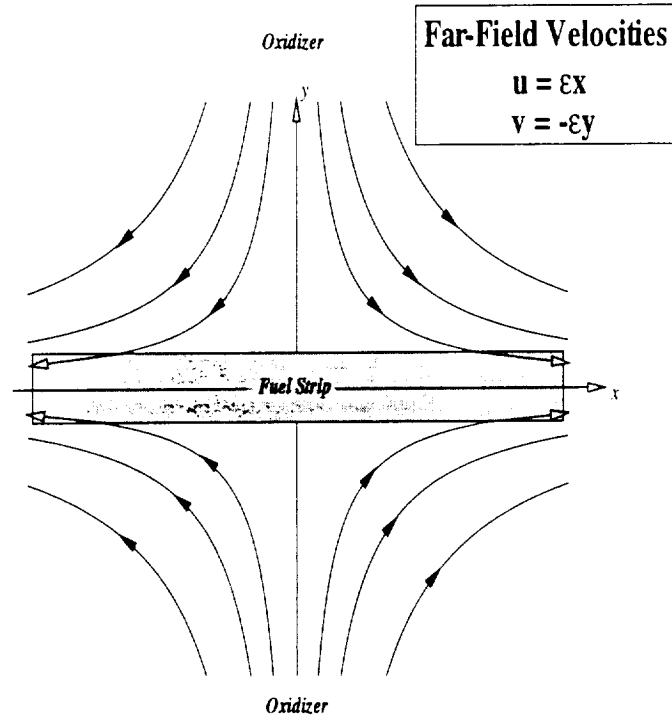


Figure 1. Geometry of strained fuel strip problem, where y_o is the initial strip thickness. The strip is exposed to the temporally evolving strain rate $\epsilon(t)$ in general.

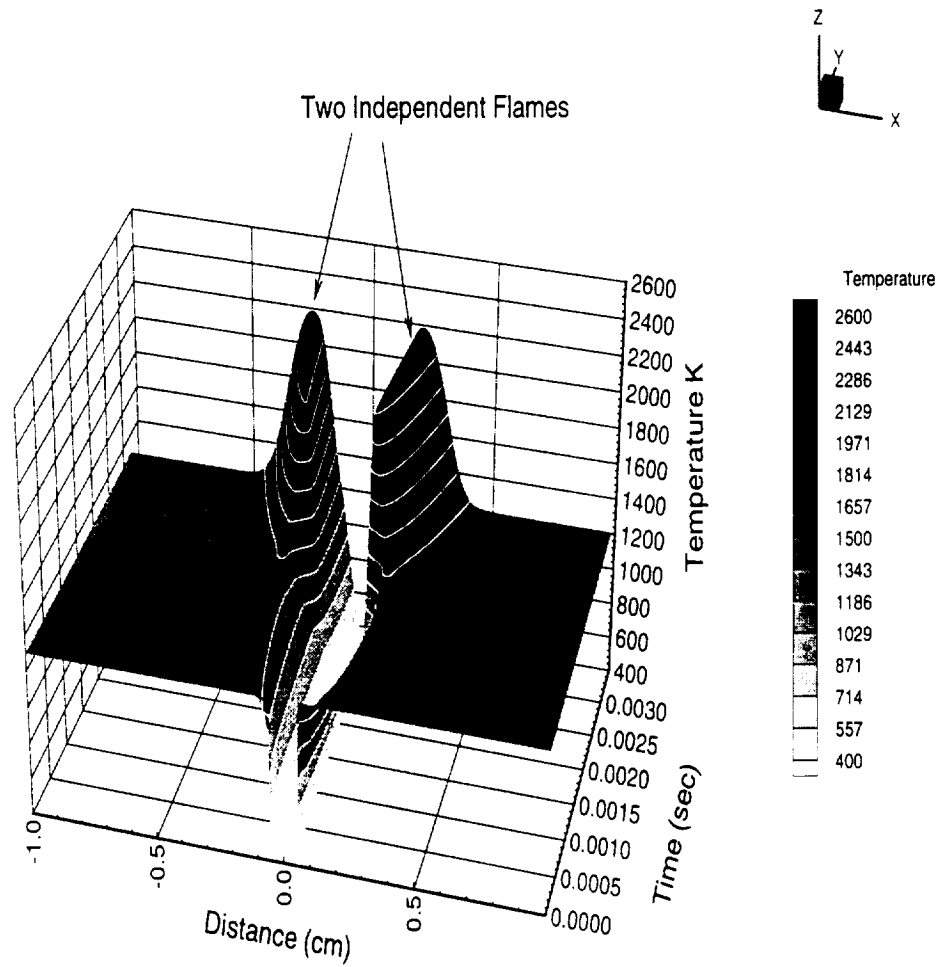


Figure 2. Temporal and spatial evolution of temperature for the unstrained fuel strip with initial thickness 1 mm. The initial temperature of fuel is 400° K and of air is 1300° K.

Two Dependent Flames

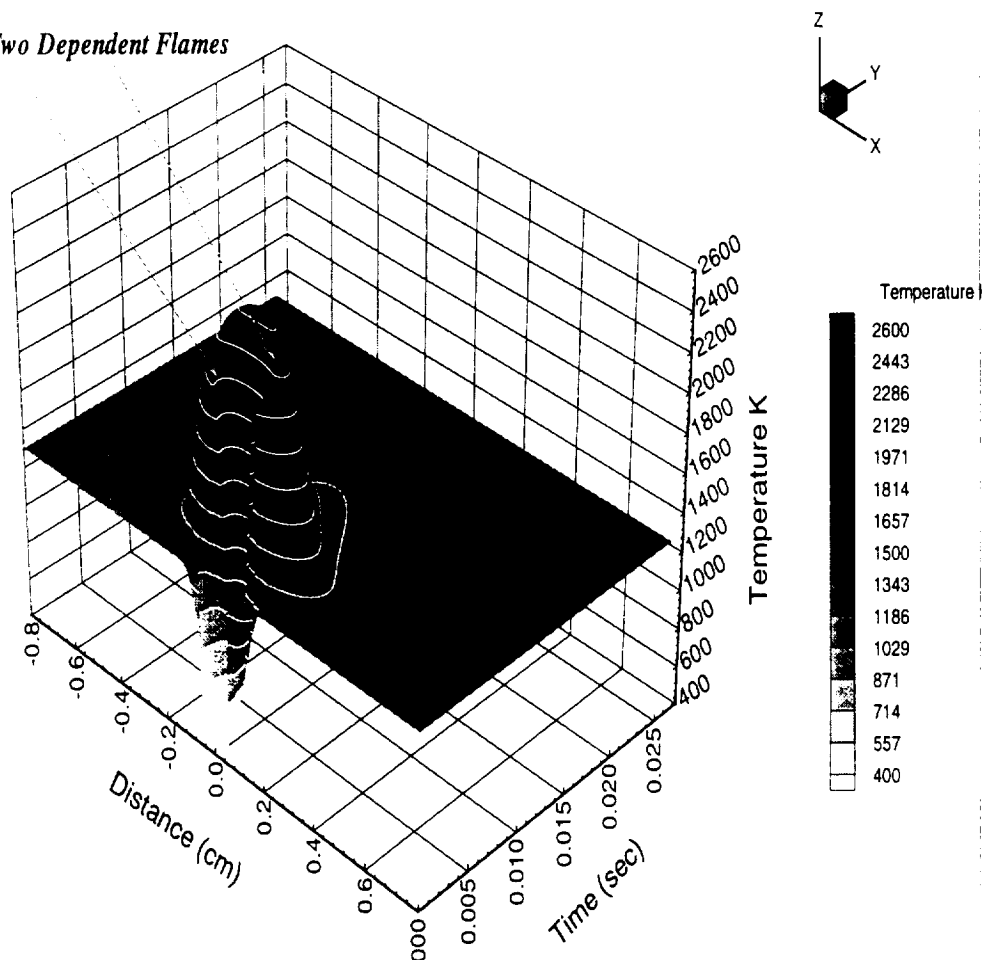


Figure 3. Temporal and spatial evolution of temperature for the strained fuel strip with initial thickness 1.0 mm and constant rate of strain 500 sec^{-1} . The initial temperature of fuel is 400° K and of air is 1300° K .

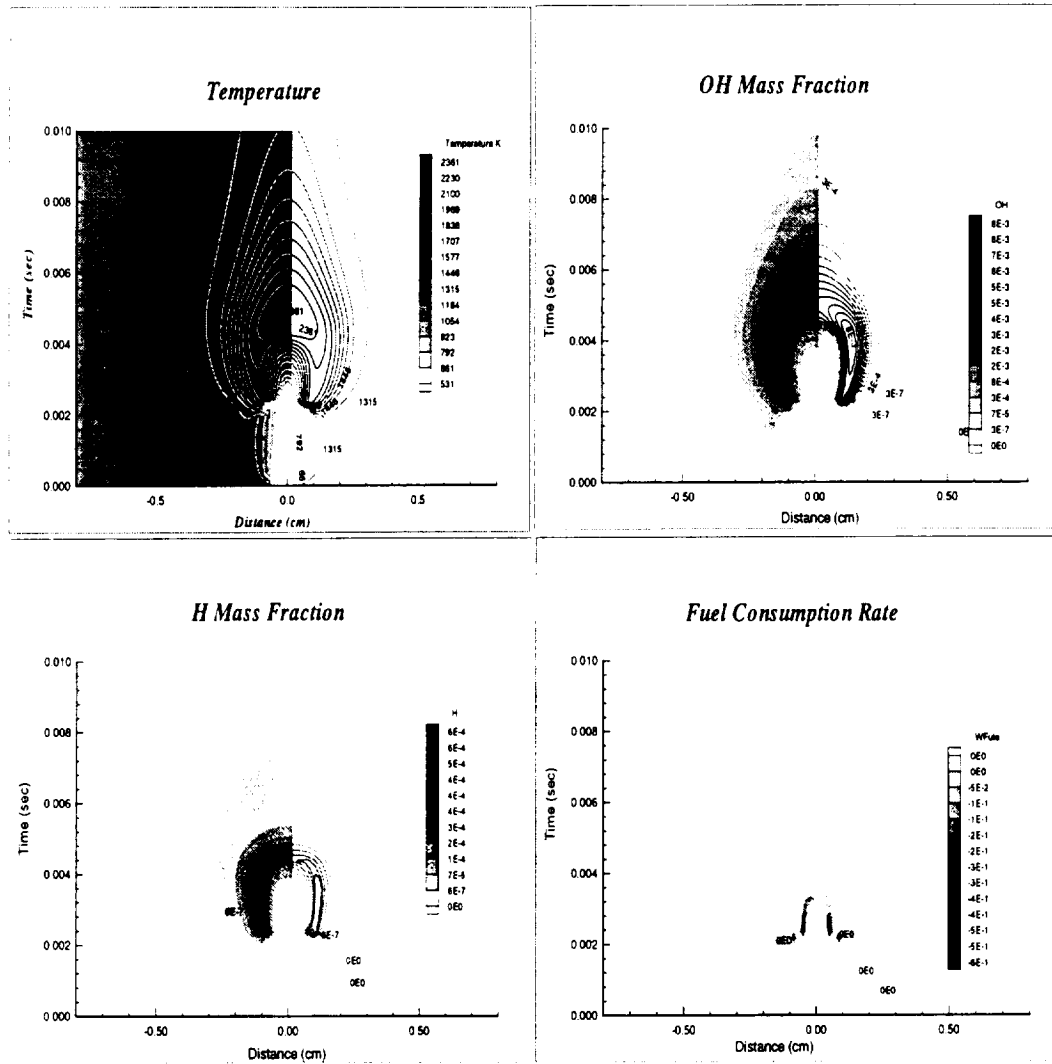


Figure 4. Temporal and spatial evolution of temperature, fuel consumption rate, OH, and H mass fractions for the strained fuel strip with initial thickness 1.0 mm and constant rate of strain 500 sec^{-1} . The initial temperature of fuel is 400° K and of air is 1300° K .

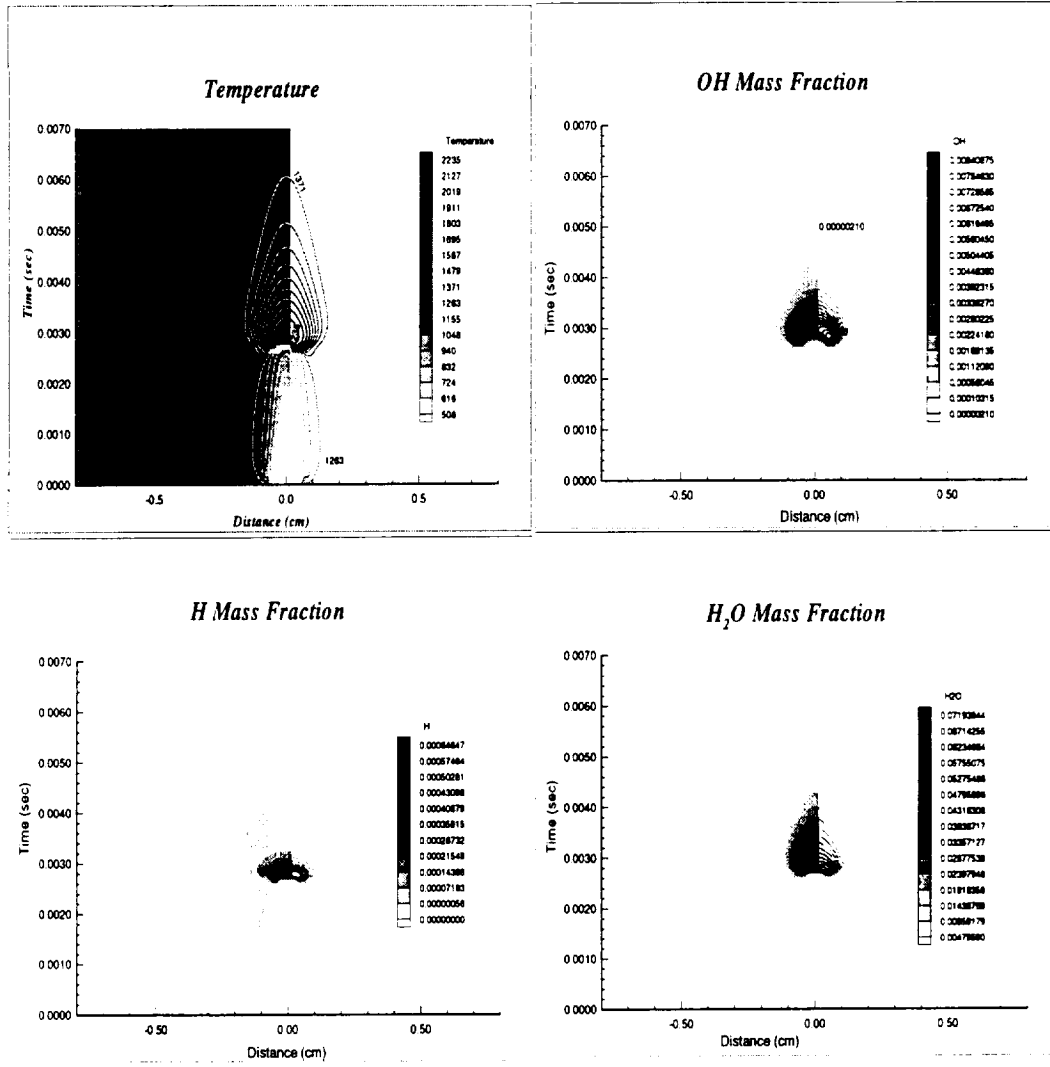


Figure 5. Temporal and spatial evolution of temperature, fuel consumption rate, OH, and H mass fractions for the strained fuel strip with initial thickness 1.0 mm and constant rate of strain 1000 sec^{-1} . The initial temperature of fuel is 400° K and of air is 1300° K .

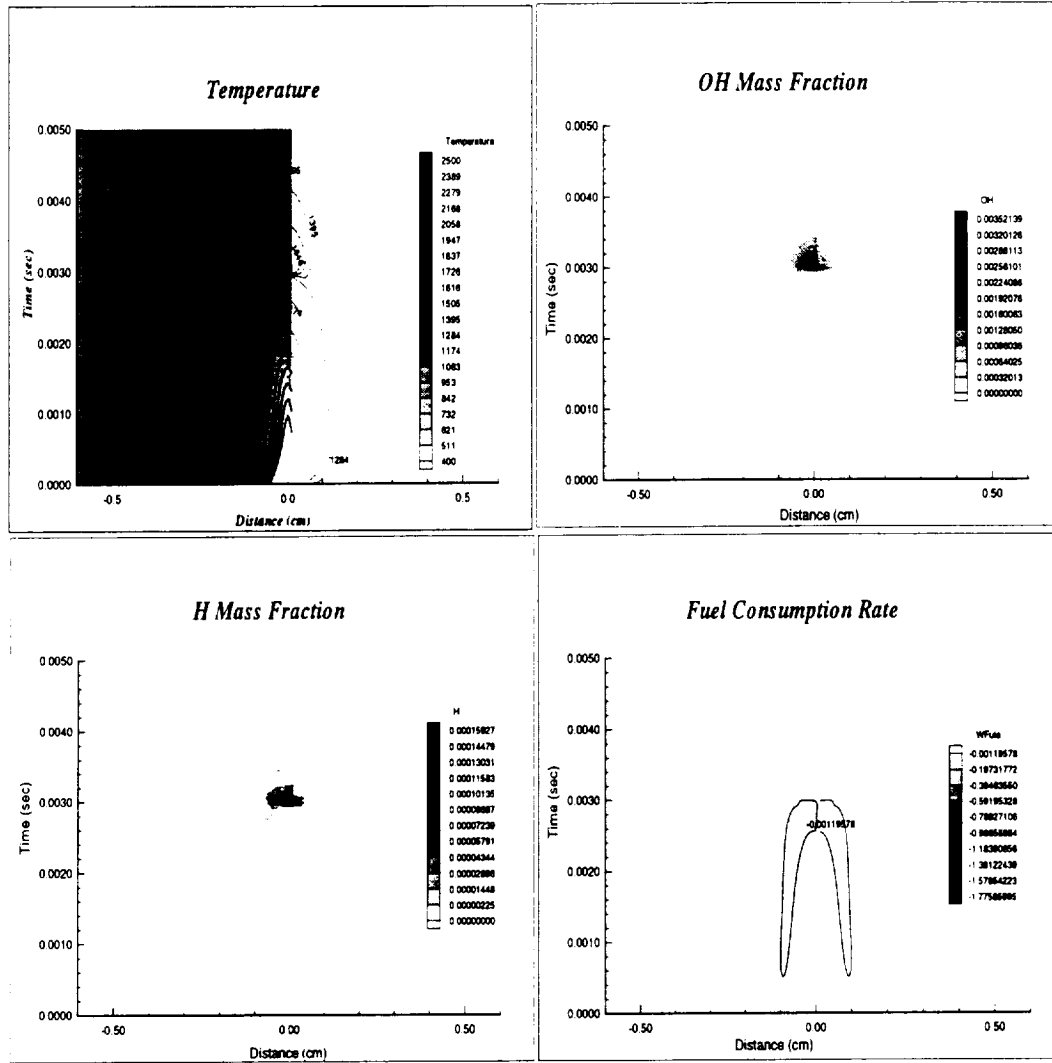
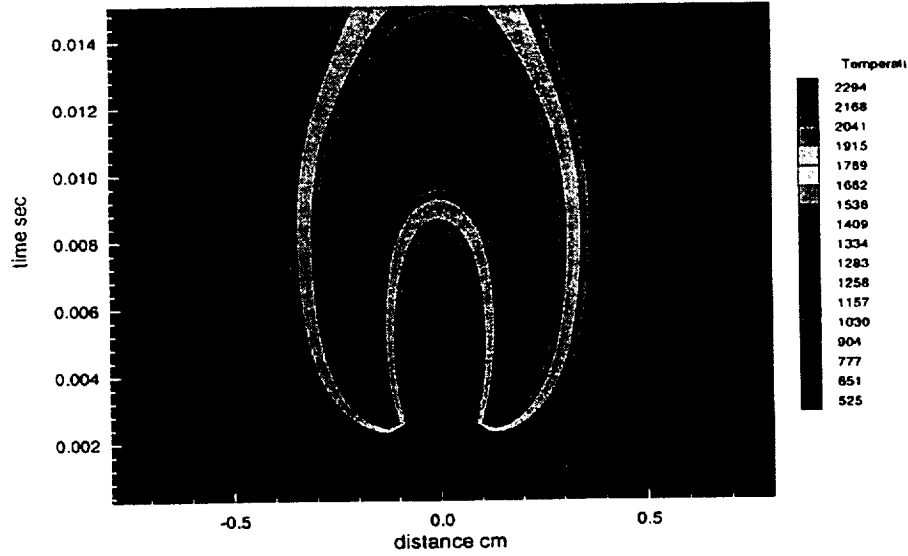


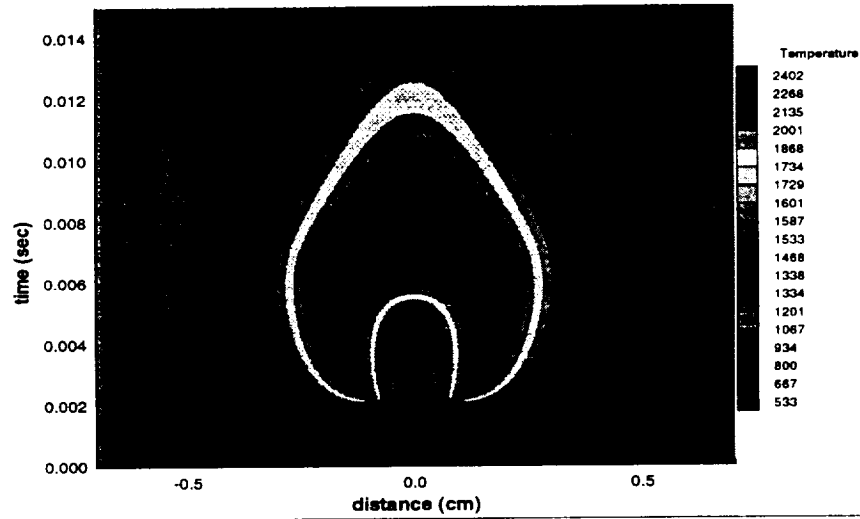
Figure 6. Temporal and spatial evolution of temperature, fuel consumption rate, OH, and H mass fractions for the strained fuel strip with initial thickness 1.0 mm and constant rate of strain 1500 sec^{-1} . The initial temperature of fuel is 400° K and of air is 1300° K .

Temperature ($st = 300$, $L = 1\text{mm}$, viscous flow)



(a) viscous case

Temperature K ($\varepsilon = 300 \text{ sec}^{-1}$, $L = 1 \text{ mm}$, inviscid flow)



(b) Inviscid case

Figure 7: Temporal and spatial evolution of temperature for the strained fuel strip with initial thickness 1.0 mm and constant rate of strain 300 sec^{-1} . The initial temperature of fuel is 400° K and of air is 1300° K .